AMENDMENTS TO THE CLAIMS

1. (Original) A molecular simulation method for dividing a molecule or a part of molecule to be simulated into a QM space and an MM apace and applying an *ab initio* molecular orbital method to the QM space and a method based on an empirical potential to the MM space to perform molecular simulation, the method comprising the steps of:

retrieving structure data on the molecule or part of molecule to be simulated from a storage unit, and dividing the structure data into the QM space and the MM space; and

replacing a part of a total energy expression in the *ab initio* molecular orbital method concerning the QM space with an empirical potential.

2. (Original) A molecular simulation method for dividing a molecule or a part of molecule to be simulated into a QM space and an MM apace and applying an *ab initio* molecular orbital method to the QM space and a method based on an empirical potential to the MM space to perform molecular simulation, the method comprising the steps of:

retrieving structure data on the molecule or part of molecule to be simulated from a storage unit, dividing the structure data into the QM space and the MM space, and dividing the QM space into a superficial QM region, which is a region adjacent to the MM space, and a QM region, which is a region except the superficial QM region;

acquiring a total energy expression in the *ab initio* molecular orbital method concerning the superficial QM region;

acquiring a total energy expression in the *ab initio* molecular orbital method concerning the QM region;

replacing a part of the total energy expression concerning the superficial QM region with a term based on the empirical potential; and

obtaining total energy in the *ab initio* molecular orbital method concerning the QM space.

3. (Original) The method according to Claim 2, further comprising the step of inputting a parameter, wherein a ratio of replacing the part of the total energy expression in the superficial QM region with the term based on the empirical potential is designated by the parameter.

4. (Original) The method according to Claim 3, wherein a plurality of superficial QM regions are set, a parameter is input for each of the superficial QM regions, and an empirical potential including Coulomb interactions and van der Waals interactions among the superficial QM regions is used.

5. (Currently Amended) The method as according to [anyone of Claims 2 to 4,] Claim 2, further comprising the step of representing a wave function in the superficial QM region by a localized molecular orbital.

6. (Original) The method according to Claim 5, further comprising the step of performing a molecule structure optimization and a time evolution calculation, wherein the localized molecular orbital is updated when the molecule structure optimization and the time expansion calculation are performed.

7. (Original) A molecular simulation device for dividing a molecule or a part of molecule to be simulated into a QM space and an MM space and applying an *ab initio* molecular orbital method to the QM space and a method based on an empirical potential to the MM space to perform molecular simulation, the device comprising:

a storage unit for storing structure data on the molecule or part of molecule to be simulated;

a region division unit for retrieving structure data on the molecule or part of molecule to be simulated from the storage unit, for dividing the structure data into the QM space and the MM space, and for dividing the QM space into a superficial QM region, which is a region adjacent to the MM space, and an QM region, which is a region except the superficial QM region; and

a first computing unit for acquiring a total energy expression in the *ab initio* molecular orbital method concerning the superficial QM region, for acquiring a total energy expression in the *ab initio* molecular orbital method concerning the QM region, for replacing a part of the total energy expression concerning the superficial QM region with a term based on the empirical

potential, and for obtaining total energy in the *ab initio* molecular orbital method concerning the QM space.

8. (Original) The device according to Claim 7, further comprising a parameter input unit for inputting a parameter, wherein the first computing unit replaces the part of the total energy expression in the superficial QM region with the term based on the empirical potential at a ratio designated by the parameter.

9. (Original) The device according to Claim 8, wherein a plurality of superficial QM regions are set, a parameter is input for each of the superficial QM reagions, and an empirical potential including Coulomb interactions and van der Waals interactions among the superficial QM regions is used.

10. (Currently Amended) The device according to [any one of Claims 7 to 9,] Claim 7, further comprising:

a second computing unit for obtaining total energy based on the empirical potential concerning the MM space; and

an output unit for calculating total energy of the molecule or part of molecule to be simulated in accordance with the total energy obtained in the first computing unit and the total energy obtained in the second computing unit.

11. (Original) A program making a computer function as

a storage unit for storing structure data on a molecule or part of molecule to be simulated;

a region division unit for retrieving structure data on the molecule or part of molecule to be simulated from the storage unit, for dividing the structure data into a QM space and an MM space, and for dividing the QM space into a superficial QM region, which is a region adjacent to the MM space, and an QM region, which is a region except the superficial QM region; and

a first computing unit for acquiring a total energy expression in an *ab initio* molecular orbital method concerning the superficial QM region, for acquiring a total energy expression in the *ab initio* molecular orbital method concerning the QM region, for replacing a part of the total energy expression concerning the superficial QM region with a term based on the empirical potential, and for obtaining total energy in the *ab initio* molecular orbital method concerning the QM space.

12. (Original) The program according to Claim 11, further making the computer function as:

a second computing unit for obtaining total energy based on the empirical potential concerning the MM space; and

an output unit for calculating total energy of the molecule or part of molecule to be simulated in accordance with the total energy obtained in the first computing unit and the total energy obtained in the second computing unit.

13. (Currently Amended) A storage medium readable by a computer in which the program according to Claim 11 [or 12] is stored.

14. (New) The method as according to Claim 3, further comprising the step of representing a wave function in the superficial QM region by a localized molecular orbital.

15. (New) The method as according to Claim 4, further comprising the step of representing a wave function in the superficial QM region by a localized molecular orbital.

16. (New) The device according to Claim 8, further comprising:

a second computing unit for obtaining total energy based on the empirical potential concerning the MM space; and

an output unit for calculating total energy of the molecule or part of molecule to be simulated in accordance with the total energy obtained in the first computing unit and the total energy obtained in the second computing unit.

17. (New) The device according to Claim 9, further comprising:

a second computing unit for obtaining total energy based on the empirical potential concerning the MM space; and

an output unit for calculating total energy of the molecule or part of molecule to be simulated in accordance with the total energy obtained in the first computing unit and the total energy obtained in the second computing unit.

18. (New) A storage medium readable by a computer in which the program according to Claim 12 is stored